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FOREWORD

This final report was submitted by the University of Dayton in support of contract F04611-83-C-0046 with the Air Force Astronautics Laboratory (AFAL), Edwards Air Force Base, CA. AFAL Project Manager was Dr Steve Rodgers.

This report has been reviewed and is approved for distribution in accordance with the the distribution statement on the cover and on the DD Form 1473.

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Calculations on the potential energy surfaces of the ground electronic state of ArH and several of its excited states, as well as the potential energy curve of ArH^+ are discussed. The need for a basis set that is both small enough to be tractable and large enough to include adequate polarizing functions to describe the long-range interaction in ground state ArH is also presented. These calculations were performed to aid in understanding the mechanisms by which energy can be stored by stabilizing a proton in a rare gas matrix. Plans for expansion of this work are discussed as is the effort expended in getting state-of-the-art molecular electronic structure algorithms to work on the Cray-2 computer.

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SUMMARY

The energy of ionization of a hydrogen atom may be stored if a proton can be stabilized in a rare gas matrix. If this is to be accomplished, the loss mechanisms resulting from dissociative recombination in the reactions

$$ArH^+ + e^- \rightarrow Ar + H^*$$

and

$$ArH^+ + e^- \rightarrow Ar^* + H$$

must be fully understood. This understanding can only be accomplished from a consistent calculation of the potential surfaces of the ArH^+, and the ground and excited states of ArH.

To perform a consistent calculation of the potential energy surfaces it is necessary to have a basis set for Ar and H which includes functions capable of describing the ground and excited states of the individual atoms, their excitation energies, and the polarizability of the atoms. The basis sets finally chosen meet our criteria. They describe the attributes of the separated atoms we are concerned with but are still small enough to be tractable. Results of calculations of the potential energy surfaces of the ground states of ArH and ArH^+ are presented for three basis sets.

Considerable effort has been expended to obtain state-of-the-art molecular electronic structure algorithms and to make them compatible with the operating system, compiler, and libraries available on the Cray-2 computer at the Air Force Supercomputer Center at Kirtland Air Force Base (AFSCC-K). Virtually all of the programs are available at the present time. More will be added as the need arises.

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INTRODUCTION

The purpose of this task is to determine viable high energy density (HED) materials for use as energy storage media in rockets. The approach is to use theoretical and computational chemistry techniques to determine what materials will have the best chance of success in meeting these goals. This report summarizes progress in the past eight months along several fronts. The technical discussion indicates the general approach in studying HED materials. That section also contains information pertaining to the ArH/ArH^+ system as a possible candidate for energy storage and the mechanism for such storage. The Results and Discussion section presents the progress made in this laboratory on the study of such of HED materials. Finally, plans for further study and conclusions are presented.

TECHNICAL DISCUSSION

All systems potentially useful as energy storage devices share a common aspect. The storage of energy is brought about by the existence of an excited state which is stable or metastable with respect to another state which is lower in energy. Thus if the excited state can be formed the excitation energy can be stored until a transition to the lower state is induced. This concept can be described schematically by the following equation:

$$A^* \text{ ---> } A + \text{energy} \quad . \tag{1}$$

Here, A^* is the excited state and A is the lower energy state. The mechanism for formation of A^* is not specified at this time, nor is the mechanism by which the decay to A is brought about. These mechanisms may be chemical or physical in nature; the mechanism is dependent on the species represented by A^* and A in Equation (1).

The key point is that to determine the mechanism we must understand the nature of A^* and A. It is just this sort of problem that theoretical and computational chemistry is well suited to solve. Modern ab initio computational chemistry programs when correctly implemented are capable of determining potential energy surfaces of a variety of chemical species as well as transition states, transition moments, and reaction pathways for chemical interactions.

The system currently being investigated makes use of the idea of employing the ionized form of an atom or molecule to store a quantity of energy equal to the ionization energy of the starting system. For example, the hydrogen atom has an ionization potential of 13.6 eV, i.e.,

$$H \text{ ---> } H^+ + e^- \qquad H = 13.6\text{eV} \quad . \tag{2}$$

Unfortunately, the proton (H^+) is "hungry" for an electron and will undergo the reverse reaction preferentially unless the proton can be stabilized and separated from electrons with which to recombine. A mechanism for stabilizing protons in a rare gas matrix was suggested by Helvagian, et al.[1] The ArH^+ ion is extremely stable with a well depth comparable to that of HCl, with

which it is isoelectronic. ArH, on the other hand, is extremely weakly bound, as is evidenced by its very small D_e and the fact that it supports no bound vibrational levels. Some of the excited states of neutral ArH, however, are quite stable relative to the ground state and could serve as intermediate states for the electron attachment process needed to release the stored energy. However, some of these excited states may also be dissociative and could serve as channels for dissociative recombination processes. Helvagian is currently working on an experimental approach to the study of the electron attachment process in ArH^+. The current theoretical approach is designed to complement that study by determining the potential energy surfaces and transition dipole moments of the ground and several excited states of ArH as well as the potential surface of ArH^+, in a computationally consistent manner, so that we may understand the bound and dissociative mechanism likely to be of concern in the ArH^+/rare gas matrix.

From a well designed calculation we can obtain a wealth of information: potential energy curves, vibrational and rotational energy levels, dipole and quadrupole moments, and transition moments. We can also obtain information about states that are difficult or impossible to investigate experimentally, for example bound and dissociating states. Thus, we can explore regions of the potential surface not otherwise accessible. Since we use computational techniques that make use of analytical potential energy derivatives, we can determine forces on atoms, stationary points on the potential surface, force constants, vibrational frequencies, zero point energies, reaction pathways, as well as the curvature of the reaction paths.

Perhaps the most important part of any quantum mechanical calculation is the basis set. All of the atomic wavefunctions are a linear combination of atomic basis functions. The size and quality of the basis set, therefore, determine the number of the molecular configurations, and thus the quality of the molecular wavefunctions and energies. Of course, if the basis set is too large the calculation is prohibitively expensive to carry out. If the basis set is too small it is not worthwhile carrying out the computation at all, since there is no chance of obtaining reliable results from an unreliable basis set.

RESULTS AND DISCUSSION

Implementation of the MESA Codes

The MESA (Molecular Electronic Structure Algorithms) codes[2] were designed and written by Byron H. Lengsfield, III and Paul Saxe at the U.S. Army Ballistic Research Laboratory (BRL) and the Los Alamos Scientific Laboratory (LASL), respectively. Since at least two thirds of my time in the last eight months has been spent getting the codes to work at the Air Force Weapons Laboratory (AFWL) supercomputer center, it seems worthwhile to discuss some of the problems encountered in transferring the programs from their source at LASL to AFWL.

The MESA codes were originally written to run on a Sun Microsystems Workstation (Sun) at LASL. The Sun is a small but extremely powerful computer which uses no extensions to the ANSI standards of FORTRAN-77. Thus a program written for a Sun should in theory be easily transportable to any other machine with only minor modifications. Specifically, the only modifications required should be in calls to library routines resident on a specific machine. Thus the Sun version of the library of subroutines will be different from the Cray-1 version. The structure of the programs themselves should not vary since the algorithms they employ remain constant across machines. The copies of the programs received from Saxe at LASL were running on the LASL Cray-1, which uses the Cray Time Sharing System (CTSS) as its operating system, the CFT FORTRAN compiler, and the machine and system library, CFTLIB. All of the codes ran with no necessary modifications on the AFWL Cray-1 computer, which also had this system configuration. Unfortunately, the Cray-1 is scheduled to become a classified machine shortly and will be unavailable for our use. Thus effecting a speedy transfer of the codes from the Cray-1 to the Cray-2 is imperative. The Cray-2 as it is configured at AFWL is different in several respects from the Cray-1; although it runs CTSS as its operating system, any similarities to the Cray-1 end there. The FORTRAN compiler on the Cray-2 is CFT77. The machine and system library is FORTLIB. Therefore all the calls to CFTLIB functions and subroutines had to be identified and changed to the analogous calls in FORTLIB. Unfortunately, however, not all of the CFTLIB routines have counterparts in FORTLIB, so changes had to be made in the MESA libraries to accommodate the missing routines.

During this time the MESA codes themselves were in a state of flux. Since they are so new, they were undergoing revision and modification even while I was trying to get the original versions going on the Cray-2. I received a second version of the codes in the middle of December and a third version of the codes in early February. During that time changes were made to the CFT77 compiler by Cray Research, Inc. I helped to identify several incompatibilities between the FORTLIB libraries and the new version of CFT77 through my efforts to get the third version of MESA working.

ArH and ArH^+ Calculations

If protons are to be stored in a rare gas matrix, it is necessary to determine mechanisms which could cause ArH^+ to capture an electron prematurely. It is also vitally important to know if protons can be stored in a rare gas matrix. There has been some discussion in the literature concerning this point.[3,4]

Milligan and Jacox[3] and Bondybey and Pimentel[4] have investigated the photolysis of hydrogen and deuterium containing molecules in argon matrices at 14K. Both groups observed absorptions at 905 cm^{-1} for hydrogen-containing systems and at 644 cm^{-1}. Milligan and Jacox attribute these absorptions to the presence of Ar_nH^+ and Ar_nD^+ species, with n equal to 2,4,.... Bondybey and Pimentel attribute the peaks to the presence of a neutral H (or D) atom in an octahedral site of argon atoms. The crux of the argument by Bondybey and Pimentel against the absorber being ArH is that this is too unstable. Furthermore, since no counter ions were observed, the absorbing specie cannot be an ion. They conclude that because of the magnitude of the D-H isotope shift the absorber must find itself in an octahedral site. Milligan and Jacox argued that there exists a large body of evidence indicating that molecular ions can indeed be trapped in argon matrices. Furthermore, the peaks at 905 cm^{-1} and 644 cm^{-1} are especially prominent in systems with known electron acceptors, and that coulombic stabilization of ion pairs in Ar lattices is appreciable. There is also mass spectrometric evidence, by Chupka and Russell[5] that Ar_2H^+ is stable. More recent work by Jacox[6] on $HCCl_3$ in Ar and Kr substantiates her arguments in favor of the presence of Ar_2H^+.

There have been several theoretical investigations of ArH[7-11] and ArH^+.[7,12] However, there has been no recent single study of the ground and low-lying excited states of ArH and the ground state of ArH^+. If we are to understand the electron attachment mechanisms of ArH^+ we must be able to investigate all of the states at the same level of approximation. The MESA codes with their ability to do complete active space self consistent field (CASSCF) and multireference determinant configuration interaction calculations (MRDCI) based on the CASSCF wavefunctions are uniquely suited to such a study.

We have performed some preliminary investigations of the ground states of ArH and ArH^+. These calculations have indicated what basis sets for Ar and H are necessary to obtain reasonable results. Our first calculations employed a very large basis for Ar, developed by Stark and Peyerimhoff[13] and a very small basis for H, developed by Huzinaga.[14] Our results, which are included in Table 1 for ArH and Table 2 for ArH^+, are unsatisfactory for ArH. This is probably due to a very large amount of basis set superposition error since the basis set for hydrogen is so much smaller than that for argon. We also investigated the efficacy of the use of the compact effective core potential and shared exponent basis sets for argon developed by Stevens, Basch, and Krauss.[15] The latter basis sets will have to be augmented with several polarization functions to give us a nearly correct binding energy for ArH.

TABLE 1. Characteristic Constants of ArH.

Source	$R_e(a_o)$	$D_e(cm^{-1})$	$\omega_e(cm^{-1})$	$\omega_e x_e(cm^{-1})$
Present[1]	6.94	216.5	107.5	13.3
Present[2]	7.75	4.8	--	--
Present[3]	6.77	67.9	--	--
Das, et al[4]	6.59	38.7	--	--
Welz[5]	6.82	33.1	--	--

1 The basis set of Ref. 13 for Ar with H basis the double zeta polarization basis of Ref. 14.
2 The basis set of Ref. 15 for Ar with H basis the double zeta plus polarization basis of Ref. 14.
3 The basis set of Ref. 16 for Ar with polarization functions of Ref. 20. The H basis is from Ref. 18.
4 Ref. 7.
5 Ref. 16.

TABLE 2. Characteristic Constants of ArH^+.

Source	$R_e(a_o)$	$D_e(cm^{-1})$	$\omega_e(cm^{-1})$	$\omega_e x_e(cm^{-1})$
Present[1]	2.44	32 828	2736	57.0
Present[2]	2.51	29 925	2736	62.5
Present[3]	2.44	33 216	2728	56.0
Matcha and Milleur[4]	2.57	21 940	2771	--
Chupka and Russell[5]	2.53	33 635	--	--

1 The basis set of Ref. 13 for Ar with H basis the double zeta polarization basis of Ref. 14.
2 The basis set of Ref. 15 for Ar with H basis the double zeta plus polarization basis of Ref. 14.
3 The basis set of Ref. 16 for Ar with polarization functions of ref. 22. The H basis is from Ref. 18.
4 Ref. 8.
5 Ref. 5.

The key in choosing the best basis set is to have sufficient polarization functions on argon and hydrogen to give the best description of the van der Waals interaction which governs the existence of the long-range potential well in ArH. These interactions are a direct result of the induced dipole-induced dipole interactions in argon and hydrogen and higher order dispersion interactions like the induced quadrupole-induced quadrupole, etc.

We have investigated a third basis set which seems to meet our criteria of being small enough to be tractable but large enough to include polarization functions necessary for a correct description of the interactions. That basis set is given in Table 3 and employs basis sets by McLean and Chandler,[17] and by Meyer.[18]

TABLE 3. The "Best" Combination of Basis Sets for Ar and H Used Used Thus Far. (See Refs. 18 and 20 for a discussion.)

Argon			Hydrogen		
Type	ζ	Contraction Coefficient	Type	ζ	Contraction Coefficient
s	118022.4	0.000747	s	68.1600	0.00255
	17683.5	0.005790		10.2465	0.01938
	4027.8	0.029919		2.34648	0.09280
	1145.40	0.119196			
	377.16	0.369096		0.673320	1.00000
	138.160	0.576399			
				0.224660	1.00000
	138.160	0.283926			
	54.989	0.622980		0.082217	1.00000
	23.171	0.283926			
			p	0.70000	1.00000
	7.3779	1.000000			
				0.20000	1.00000
				0.07000	1.00000
	0.6504	1.000000			
			d	0.20000	1.00000
	0.2328	1.000000			
				0.07000	1.00000
	0.08	1.000000			
p	663.06	0.003042			
	157.09	0.023949			
	50.231	0.107088			
	18.635	0.291873			
	7.4465	0.452621			
	3.0957	0.308483			
	1.1065	1.000000			
	0.4156	1.000000			
	0.1454	1.000000			
	0.0500	1.000000			
d	1.000000	1.000000			
	0.3	1.000000			
	0.1	1.000000			

Our results thus far are quite rudimentary. We have performed first-order configuration interaction calculations of ArH and ArH^+ using a wavefunction obtained from a Hartree-Fock single configuration self-consistent field calculation. Our results employing the third basis set are in quite good agreement with results from other calculations and from experiment.[19] The earliest calculations[6,7] were performed at a rather high level of approximation with relatively small basis sets. Those results are subject to basis set superposition errors which may cancel the effects of the high degree of approximations made. This fortuitous cancellation of errors may explain the excellent agreement between those results and experiment. It is, however, clear from our results that the specie whose absorption was observed in the argon matrix studies is neither ArH nor ArH^+.

CONCLUSIONS AND RECOMMENDATIONS

To meet our goal of characterizing the ground and excited states of ArH and the ground state of ArH^+ at a consistent level of calculation, we must calculate the potential energy surfaces based on a CASSCF approach. Then we will be able to determine the transition dipole moment functions and radiative lifetimes of the excited states of ArH with respect to the ground state. At that stage we will be able to approach the determination of the electron attachment process in ArH^+.

At that point we will be able to go on to determine the potential energy surfaces of Ar_2H, Ar_4H, Ar_2H^+, and Ar_4H^+. At that point we hope to be able to determine which species were most probably observed by Milligan and Jacox and Bondybey and Pimentel and to judge whether indeed it will be possible to store the ionization energy of hydrogen in a rare gas matrix.

If it becomes necessary to investigate Ar_nH and Ar_nH^+ clusters with n larger than 4, we will have to return to the idea of using compact effective core potentials[15] and other approaches. One such approach may be to use the Reaction Field technique developed by Stevens.[21] The Reaction Field operates analogously to the effective core potential. The latter replaces the core electrons of a molecule, which are generally not involved in bonding, with an effective core Hamiltonian. The former employs an effective Hamiltonian to replace environmental molecules which are not directly involved in the bonding region of the cluster. Also of concern is the role of dispersion forces in clusters. I intend to extend a method proposed[22] for calculating the dispersion energy including the damping effects of charge overlap for atom-diatom interactions to general molecule-molecule interactions. This work will be done in collaboration with J. Bohr, a NRC postdoctoral associate working with the HEDM theory group.

A further area which requires study is making the MESA codes even more efficient than they already are by making use of the multitasking aspects of the Cray-2. This would require amending the code to include Cray multitasking directives.

In addition to the two items already mentioned, it will be necessary to begin investigating hydrides in lighter rare gas matrices, like Ne and He. Fortunately there is a great deal more information on these systems already in the literature from which to gather ideas on approaches to the problem. Extensions of our theoretical approach to the investigation of rare gas halides in rare gas matrices must also be made. We also intend to investigate the use of substrates other than the rare gases (e.g. N_2, CO) to stabilize high energy density materials.

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